201-15259A

Testing Rationale

Carbamodithioic acid, dibutyl-,methylene ester

CAS Registry Number 10254-57-6

March 2004

Summary

The R. T. Vanderbilt Company, Inc. is pleased to submit this test plan for Carbamodithioic acid, dibutyl-,methylene ester (Vanlube® 7723) for review and public comment under the Environmental Protection Agency's High Production Volume (HPV) Challenge Program.

Vanlube® 7723 is a general purpose, ashless antioxidant which should find application in petroleum lubricants of all types. We propose the following studies to meet the requirements of the EPA High Production Volume Chemical Testing Program:

Physical/chemical properties: No testing proposed

Environmental fate: No testing proposed

Environmental toxicity: No testing proposed

Mammalian toxicity: In vitro chromosome aberration assay

BACKGROUND

Background Information: Manufacturing and Commercial Applications

Manufacturing

Vanlube 7723 has been manufactured since 1977. It is manufactured by batch rather than continuous process. Vanlube 7723 process is confidential.

Commercial Applications

Carbamodithioic acid, dibutyl-,methylene ester (VANLUBE 7723) is a general purpose, ashless antioxidant which should find application in petroleum lubricants of all types. It is effective at economical concentrations, readily soluble, and easy to blend. VANLUBE 7723 has been tested in a variety of base stocks commonly used in compounding turbine, hydraulic and circulating oils. In addition to being an effective antioxidant, VANLUBE 7723 also exhibits good extreme pressure performance alone and in combination with other additives. This material is useful as a component of additive packages.

Shipping/Distribution

Vanlube 7723 is shipped extensively throughout the world from manufacturing plants located in North America.

Worker/Consumer Exposure

To the best of our knowledge, all Vanlube 7723 is used by the lubrication additive industry, mostly by large industrial users as a component of their petroleum oil lubricating compounds. This additives industry has a long safety record and only sophisticated industrial users handle this material. It is only available as a liquid and most large industrial users have mechanized materials handling systems, so employee exposure is minimal. The greatest potential for skin and inhalation exposure is at the packing station at the manufacturing site and, to a lesser extent, during weighing activities at the customer site.

Consumer exposure is very minimal. The usage level is less than 5 weight percent in the lubricating fluid formulations.

Background Information: HPV Endpoints

Physical chemical properties

The physical chemical properties of carbamodithioic acid, dibutyl-,methylene ester have not been determined. EPIWIN modeling was used to predict boiling point, vapor pressure, and melting point of this material. Carbamodithioic acid, dibutyl-,methylene ester is not water soluble, such that

determination of the partition coefficient is not applicable. An estimated partition coefficient value is provided. Table 1 presents the physical chemical data for this material.

No additional physical/chemical properties testing is proposed.

Environmental Fate

This water-insoluble material does not appear to be readily hydrolysable, as it does not contain common hydrolysable organic functional groups such as carboxyl esters, nitriles and imines (see Figure 1) and as such hydrolysis data are not applicable. The photodegradation half-life was estimated using EPIWIN; the half-life is predicted to be 27 minutes. This material is not readily biodegradable. Fugacity modeling indicates this material would be found primarily in sediment and soil, which is consistent with its low water solubility. Table 1 presents the environmental fate data for this material.

No additional environmental fate testing is proposed.

Environmental Effects

The acute aquatic toxicity of this material is well characterized. This material has a low water solubility, and this property is characterized in the results of the testing. There was no toxicity to any organism tested (fish, daphnia or algae) at the limit of water solubility.

Additional aquatic toxicity testing is not proposed.

Mammalian Toxicity

Table 1 presents the mammalian toxicity data for this material.

Acute Toxicity: The acute oral LD_{50} for carbamodithioic acid, dibutyl-,methylene ester is 16000 mg/kg. The acute dermal LD_{50} is greater than 2,000 mg/kg.

Repeated Dose/Reproductive/Developmental Effects: A repeat dose toxicity study with screening reproductive and developmental endpoints (OECD 422) has been conducted with the test substance. The parental NOAEL was 1000 ppm; the NOAEL for F1 offspring was greater than 20000 ppm.

No additional mammalian toxicity tests are proposed.

Genotoxicity: An salmonella/mammalian-microsome plate incorporation mutagenicity assay has been conducted with carbamodithioic acid, dibutyl-,methylene ester. The results of the bacterial mutagenicity test were negative.

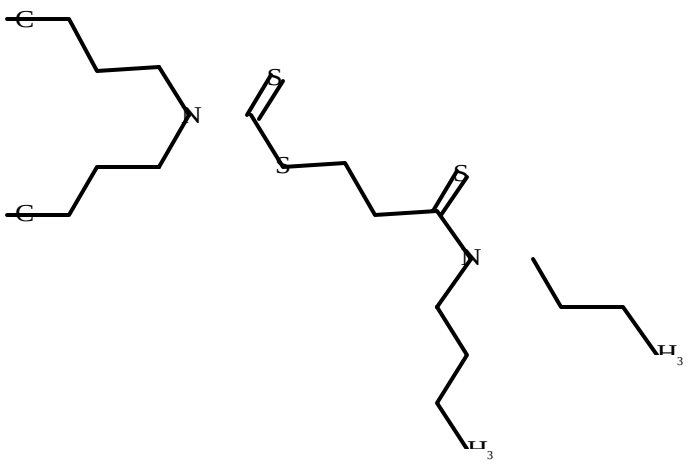
An in vitro chromosome aberration assay is proposed.

Table 1. Matrix of Available and Adequate Data

Test	CAS No. 10254-57-6
Chemical/physical Properties	
Melting Point	203 C (estimated)
Vapor Pressure	6E-10 mm Hg (estimated)
Boiling Point	490 C (estimated)
Partition Coefficient	6.73 (estimated)
Water Solubility	Not soluble (estimated .04 mg/L @ 25 C)
Environmental Fate	
Hydrolysis	No hydrolysable functional groups
Photodegradation	t1/2 = .5 hours
Biodegradation	21% in 28 days
Environmental Transport	Air 0.147% Water 13.2% Soil 32.1% Sediment 54.5%
Aquatic Toxicity	
Acute Fish 96 hr LC50	>0.06 mg/L
Acute Daphnid 48 hr EC50	>0.052 mg/L
Algae 72 hr EC50	>0.0325 mg/L
Mammalian Toxicity	
Acute Oral	16000 mg/kg (rat)
Acute Dermal	>2000 mg/kg (rabbit)
Repeated Dose	NOAEL = 1000 ppm
Genotoxicity (*in vitro* -bacteria)	negative
Genotoxicity (*in vitro mammalian*)	-
Reproductive/Developmental	NOAEL F1 offspring >20000 ppm

(-) = No data available, or data considered inadequate

Figure 1 Carbamodithioic acid, dibutyl-,methylene ester structure



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Test Plan

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Physical-Chemical				
Melting Point	**Boiling Point**	**Vapor Pressure**	**Partition Coefficient**	**Water Solubility**
Calc	Calc	Calc	Calc	A

Environmental Fate			
Photodegradation	**Stability in Water**	**Transport/ Distribution**	**Biodegradation**
Calc	NA	Calc	A

Ecotoxicity		
Acute Toxicity to Fish	**Acute Toxicity to Aquatic Plants (e.g., Algae)**	**Acute Toxicity to Aquatic Invertebrates (e.g., Daphnia)**
A	A	A

Mammalian Toxicity					
Acute Toxicity	**Bacterial Genetic Toxicity *In Vitro***	**Mammalian Genetic Toxicity *In Vitro***	**Repeat Dose Toxicity**	**Reproductive Toxicity**	**Developmental Toxicity**
A	A	Test	A	A	A

Legend	
Symbol	**Description**
Test	Endpoint requirements to be fulfilled with testing
Calc	Endpoint requirement fulfilled based on calculated data
A	Endpoint requirement fulfilled with adequate existing data
NA	Not applicable; no hydrolysable functional groups